Glutaric acid, 3,4-dimethylcyclohexyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C16H25F3O4/c1-10-7-8-13(9-11(10)2)23-15(21)6-4-5-14(20)22-12(3)16(17,18)

InchiKey: RBZQFKVTZURINZ-UHFFFAOYSA-N

Formula: C16H25F3O4

SMILES: CC1CCC(OC(=O)CCCC(=O)OC(C)C(F)(F)F)CC1C

Mol. weight [g/mol]: 338.36

Physical Properties

Property code	Value	Unit	Source
gf	-959.00	kJ/mol	Joback Method
hf	-1451.89	kJ/mol	Joback Method
hfus	35.05	kJ/mol	Joback Method
hvap	65.20	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.019		Crippen Method
mcvol	245.630	ml/mol	McGowan Method
pc	1444.64	kPa	Joback Method
rinpol	1737.00		NIST Webbook
rinpol	1737.00		NIST Webbook
tb	722.41	K	Joback Method
tc	909.80	K	Joback Method
tf	402.49	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.30	J/mol×K	722.41	Joback Method
cpg	777.29	J/mol×K	753.64	Joback Method
cpg	794.16	J/mol×K	784.87	Joback Method
cpg	809.93	J/mol×K	816.10	Joback Method
cpg	824.62	J/mol×K	847.33	Joback Method
cpg	838.24	J/mol×K	878.56	Joback Method
cpg	850.82	J/mol×K	909.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405427&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume